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COUPLED THERMAL/CHEMICAL/MECHANICAL MODELING OF ENERGETIC MATERIALS IN ALE3D(U)

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We must improve our ability to model the processes involved with the response of energetic materials to thermal stimuli. Traditionally, these analyses have involved coupled thermal transport/chemical reaction codes. This provides only a reasonable estimate of the time and location of ensuing rapid reaction. To predict the violence of the reaction, the mechanical motion must be included in the wide range of time scales associated with the thermal hazard. The ALE3D code has been modified to assess the hazards associated with heating energetic materials in weapons. We have merged the thermal transport models from TOPAZ3D and the thermal chemistry models developed in Chemical TOPAZ into ALE3D. We have developed and use an implicit time step option to handle the hours that the energetic material can take to react. Since on these longer time scales materials can be expected to have significant motion, it is even more important to provide high-order advection for all components, including the chemical species. We will show an example cook-off problem to illustrate these capabilities.

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